

# Compilation of Energy Band Gaps in Elemental and Binary Compound Semiconductors and Insulators

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Energy band gaps are tabulated for elemental and binary compound semiconductors and insulators reported in 723 references. The method of measurement, transition, type of sample, and other pertinent information are included for each entry. The determinations believed to be the most reliable are indicated.

Key words: Band gaps; binary compounds; electronic properties; insulators; semiconductors.

## 1. Introduction

This compilation of energy band gaps in elemental and binary compound semiconductors and insulators is intended for scientists who are concerned with energy states and electronic properties of solids and for materials engineers who are concerned with the application of solid state science to semiconductor device technology. Binary compounds included in this compilation are those involving elements in Groups IIIA, IVA, VA, VIA, and VIIA of the Periodic Table with elements of atomic numbers 3 (lithium) through 92 (uranium). In addition to the band gap, the compilation gives the method of measurement, the form of the sample, and the temperature at which the measurement was made for each material listed. When available, temperature coefficients of band gaps and indications of whether the material exhibits cathodoluminescence, electroluminescence, laser emission, mechanical luminescence, photoluminescence, or thermoluminescence are also given.

The data tabulated in this report were obtained from the files of the Electronic Properties Information Center (EPIC), Hughes Aircraft Company, Culver City, California, and from the Research Materials Information Center (RMIC), Oak Ridge National Laboratory, Oak Ridge, Tennessee. Additional data were extracted from Chemical Abstracts, published by the American Chemical Society, and from the open literature. An effort has been made to cover the literature through 1971.

## 2. Energy Band Gaps

According to the band theory of solids [1, 2, 3],<sup>1</sup> when atoms are brought together to form a crystal, the discrete electronic energy states of the isolated atoms merge into energy bands which represent the allowed energies for electrons in the crystal. These bands may be separated by forbidden regions or gaps. The conductivity of a solid, and hence its classification as a metal, semiconductor, or insulator, depends upon the distribution of electrons in the allowed energy bands. Electrons contained in a filled band make no contribu-

tion to the electrical conductivity. Thus, if the valence electrons exactly fill one or more bands leaving others empty, the crystal will be an insulator; if the valence electrons partially fill one or more bands the crystal will be a conductor. In an insulator at temperatures above 0 K, some electrons from the highest valence band are thermally excited into the lowest empty band and conduction becomes possible (intrinsic semiconduction). The number of electrons excited into the conduction band is a function of both the temperature and the magnitude of the energy band gap  $E_g$ , which is defined as the separation between the maximum energy in the valence band and the minimum energy in the conduction band. If  $E_g$  is small (0–3 or 4 eV) a material is considered to be a semiconductor and if  $E_g$  is large (4–12 eV) a material is considered to be an insulator. As the electrical and optical properties of a semiconductor are dependent upon the energy gap, these data are important in semiconductor device design.

Attempts have been made to correlate band gaps with other properties of the solids or with properties of the constituent elements in the solid. Correlations have been proposed between band gaps and heats of formation [4, 5], heats of atomization [6], reciprocal bond length [7], the ratio of bond length to cation radius [8], single bond energies [9], average bond energies [10], electronegativities [11], and atomic numbers [12, 13, 14]. None of these correlations yields empirical relations which are sufficiently general to be of practical use. This may be attributed in part to the number of compounds for which energy band gaps were known at the time the correlations were proposed. Winkler [15], lists only about 90 inorganic compounds which, in 1955, were known to exhibit semiconductor properties.

## 3. Measurement of Energy Band Gaps

Band gaps have been measured by both spectroscopic and conductivity methods. They have been determined from absorption and reflectance spectra [16], from photoconductivity measurements [17], and from the thermal activation energies in electrical conductivity measurements [18]. Absorption edge measurements account for a majority of the band gaps listed in this compilation.

In determining a band gap by absorption spectroscopy, the absorption coefficient,  $\alpha$ , is measured as a function of energy from below to above the absorption edge. At

<sup>1</sup> Numbers in brackets indicate references in section 6.

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the absorption edge  $\alpha$  rises steeply above background and may change by a factor of  $10^7$  in an energy range of 0.3–0.6 eV. The threshold energy,  $E_g$ , is determined by extrapolating the linear portion of the  $\alpha$  vs energy curve to a value of  $\alpha$  which is estimated or assumed to represent background. Some workers take the absorption edge to be the energy value which corresponds to a preselected value of  $\alpha$  (usually between 1 and  $100 \text{ cm}^{-1}$ ) while other workers attempt to correct for actual background. Often, the original reference does not specify the experimental procedures with sufficient detail to permit a precise comparison of results obtained by other workers. Consequently, when two or more values for a particular band gap are available, whether they have been measured by the same method or by different methods, an attempt has been made to classify the degree of reliability of the values. This classification takes into consideration the material, the method of measurement, the reported sample purity, and the experimental conditions. A review of the band gap data compiled shows that the actual experimental uncertainties are frequently greater than 5 percent and seldom less than 1 percent.

#### 4. Arrangement of Table

The energy band gap table consists of 1504 entries. Entry numbers are given at the left hand side of the table; they are cited in the author cross index. Tabulated data and comments are arranged in columns and the numbers assigned at the top of the columns denote the following:

- Column
- 1 Chemical symbol of the first elements
  - 2 Stoichiometry of the first element
  - 3 Chemical symbol of the second element
  - 4 Stoichiometry of the second element
  - 5 Band gap
  - 6 Temperature at which the quoted band gap was measured
  - 7 Temperature dependence of the band gap  
e denotes 10 raised to the indicated power
  - 8 Reliability rating:  
"1" selected as the most reliable measurement for the band gap listed  
"2" denotes other citations for the same compound
  - 9 Method of determination:  
0 Not specified  
1 Reflection  
2 Absorption  
3 Photoconduction  
4 Thermal activation  
5 Electoreflexion  
6 Magnetoabsorption  
7 Magnetoreflexion  
8 Others  
9 Estimated

10 Type of sample the band gap was determined on:

- 0 Not specified
- 1 Thin film, single crystalline
- 2 This film, polycrystalline
- 3 Single crystalline
- 4 Polycrystalline
- 5 Amorphous
- 6 Other

11 Transition involved:

First entry denotes:

- U = Unspecified transition  
E = Excitonic transition  
D = Direct transition  
I = Indirect transition

If applicable, second entry denotes:

- A = Allowed transition  
F = Forbidden transition

If applicable, third entry denotes:

- D = Direct transition is the lowest transition  
I = Indirect transition is the lowest transition

12 Selected effects reported in the citation:

- C = Cathodoluminescence  
E = Electroluminescence  
L = Laser emission  
M = Mechanical luminescence  
P = Photoluminescence  
T = Thermoluminescence

13 Color

14 Bibliographic reference number

15 Comments

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### Note

This material was originally compiled by Minnesota Mining and Manufacturing Company, St. Paul, Minnesota.